

# Chi H. Mak

## University of Southern California

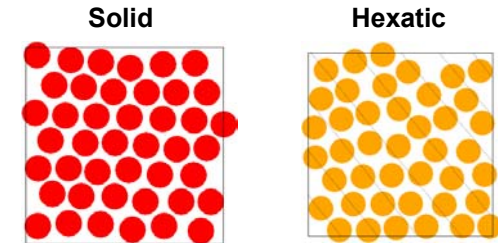
### CHE-9970766

#### Bigger Is Better!

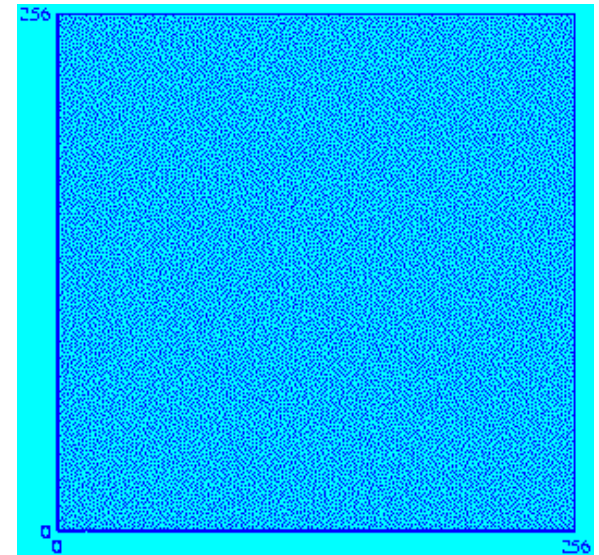
What do you get when you lay a large number of hockey pucks on a flat floor? At high density, they are packed together and you will get a crystalline solid. At lower density you get a liquid, and at still lower density, a gas. This so-called “hard disk fluid” is the simplest atomic model for phase transitions.

While the three phases of matter – solid, liquid and gas – are well known, a little-known fourth phase of matter, nicknamed the “hexatic”, has been predicted by Halperin and Nelson in 1978 for the hard disk fluid but has never been confirmed. Using large-scale computer simulations on a supercomputer, Prof. Chi Mak at the University of Southern California has finally identified this elusive hexatic phase in the hard disk fluid.

The very first simulation of a fluid was carried out back in 1959 by Alder and Wainwright using 870 hard disks. Since then, increasingly larger simulations have been performed with up to 65,000 hard disks, but none was able to identify the hexatic phase. Using more than a million hard disks, Prof. Mak’s simulations were finally able to confirm all the predictions of Halperin and Nelson, proving that at least for hockey pucks, a bigger simulation is indeed better.



Unlike the solid, the hexatic phase is noncrystalline, but the disks are lined up along a preferential direction (indicated by the parallel dotted lines).



Snapshots illustrating the motions of disks during the simulation inside a  $1/4 \times 1/4$  section of the box, showing about 65,000 of the one million particles.